

2-(propan-2-yl)-1,3,6-trioxocane
15351-38-9 | DTXSID80279934

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 65.8 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.10e-01

Confidence level: 6.99e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Urea, (3-methylphenyl)-</div> <div>Measured: 36.3</div> <div>Predicted: 37.2</div>	<div>Image not found</div> <div>Metaldehyde acetaldehyde tetramer</div> <div>Measured: 240</div> <div>Predicted: 148</div>	<div>Image not found</div> <div>N-Methyl-N'-phenylurea</div> <div>Measured: 19.5</div> <div>Predicted: 29.8</div>
<div>Image not found</div> <div>N-(3-chlorophenyl)-N'-methylurea</div> <div>Measured: 85.1</div> <div>Predicted: 101</div>	<div>Image not found</div> <div>3-Chlorophenylurea</div> <div>Measured: 102</div> <div>Predicted: 57.3</div>	